



Sample name: **M02_octanol** Experiment start time: **12/14/2017 9:40:49 PM**
Assay name: **pH-metric high logP** Analyst: **Dorothy Levorse**
Assay ID: **17L-14020** Instrument ID: **T311053**
Filename: **G:\OpenLab_PFA_Sirius-T3-1\Sirius-T3-1\Data2017\17L-14020_M02_octanol_pH-metric high logP.t3r**

pH-metric Result

logP (XH +) 1.38
logP (neutral X) 4.32
RMSD 0.298

17L-14020 Points 1 to 14

M02_octanol concentration factor 0.941
Carbonate 0.0792 mM
Acidity error 0.00723 mM

17L-14020 Points 15 to 31

M02_octanol concentration factor 0.825
Carbonate 0.1960 mM
Acidity error 0.05972 mM

17L-14020 Points 32 to 50

M02_octanol concentration factor 0.307
Carbonate 0.2201 mM
Acidity error 0.61969 mM

Warnings and errors

Errors None
Warnings None

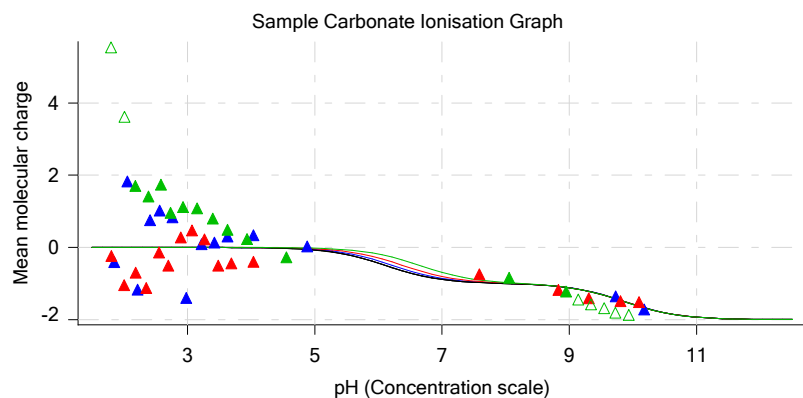
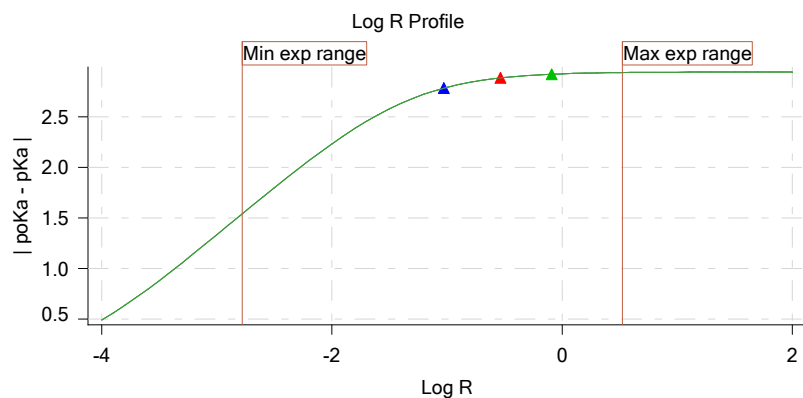
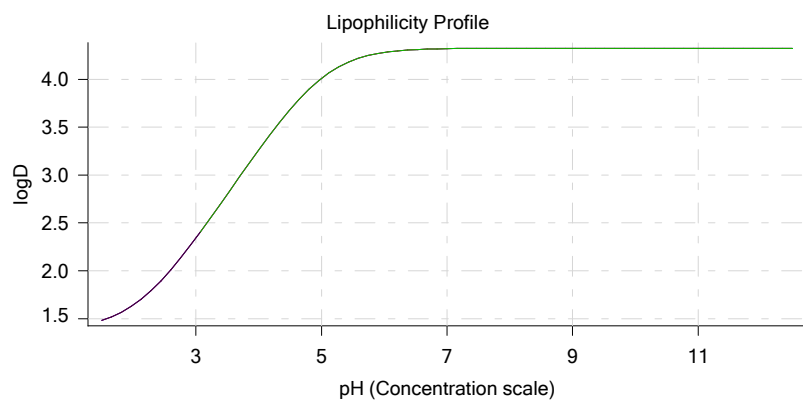
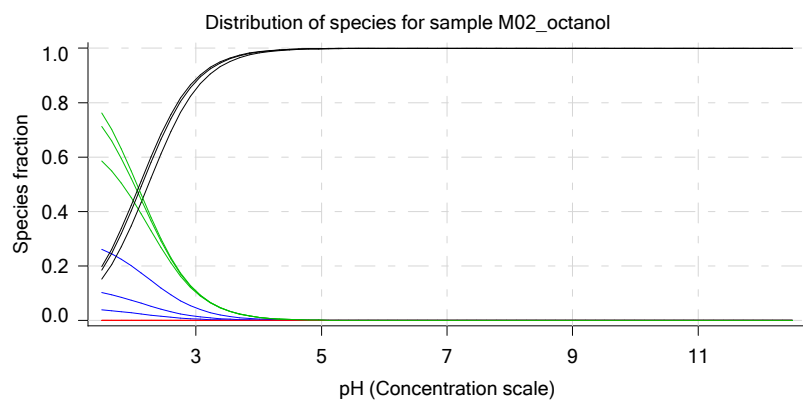
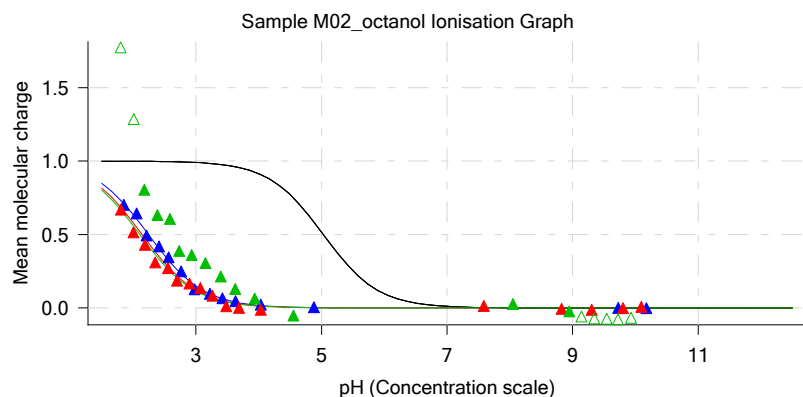
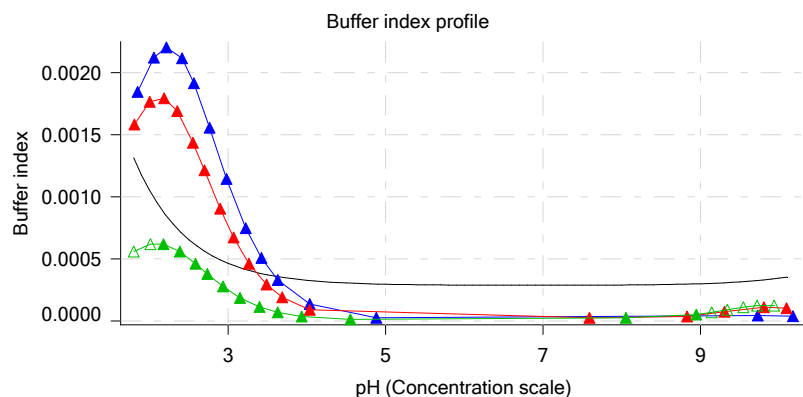
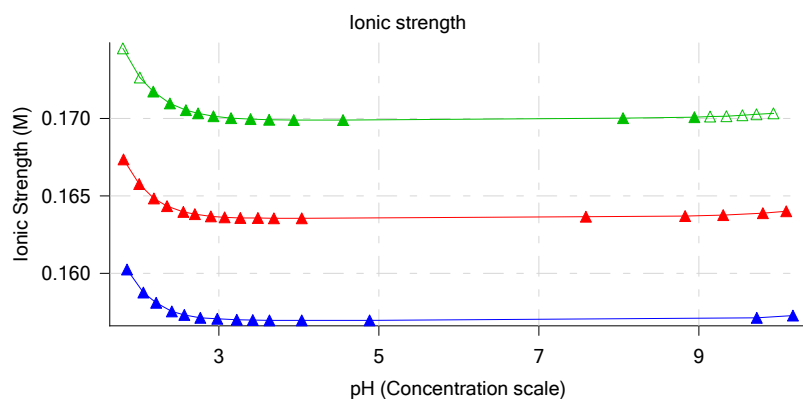
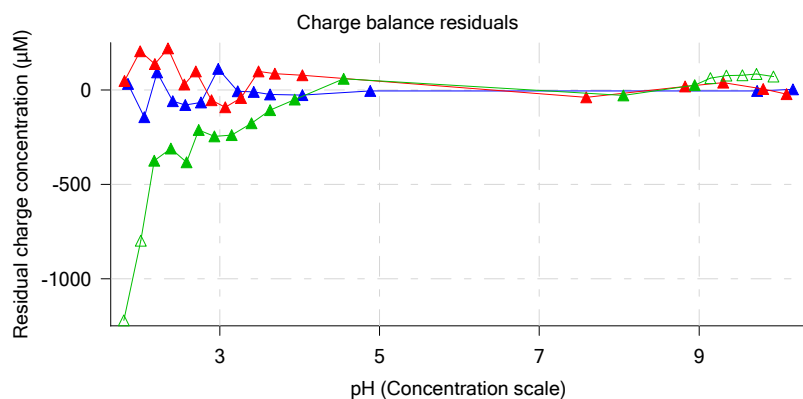
Sample logD and percent species

pH	M02_octanol logD	M02_octanol M02_octanolH	M02_octanol M02_octanol	M02_octanol M02_octanolH*	M02_octanol M02_octanol*	Comment
1.000	1.41	3.71 %	0.00 %	88.98 %	7.31 %	Stomach pH
1.200	1.43	3.56 %	0.00 %	85.33 %	11.11 %	
2.000	1.64	2.24 %	0.00 %	53.67 %	44.09 %	
3.000	2.34	0.45 %	0.00 %	10.80 %	88.74 %	
4.000	3.26	0.05 %	0.00 %	1.20 %	98.74 %	
5.000	4.01	0.01 %	0.00 %	0.12 %	99.87 %	Blood pH
6.000	4.28	0.00 %	0.00 %	0.01 %	99.98 %	
6.500	4.31	0.00 %	0.00 %	0.00 %	99.99 %	
7.000	4.32	0.00 %	0.00 %	0.00 %	99.99 %	
7.400	4.32	0.00 %	0.00 %	0.00 %	99.99 %	
8.000	4.32	0.00 %	0.00 %	0.00 %	100.00 %	
9.000	4.32	0.00 %	0.00 %	0.00 %	100.00 %	
10.000	4.32	0.00 %	0.00 %	0.00 %	100.00 %	
11.000	4.32	0.00 %	0.00 %	0.00 %	100.00 %	
12.000	4.32	0.00 %	0.00 %	0.00 %	100.00 %	

Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **17L-14020**
 Filename: **G:\OpenLab_PFA_Sirius-T3-1\Sirius-T3-1\Data2017\17L-14020_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **12/14/2017 9:40:49 PM**
 Analyst: **Dorothy Leverse**
 Instrument ID: **T311053**

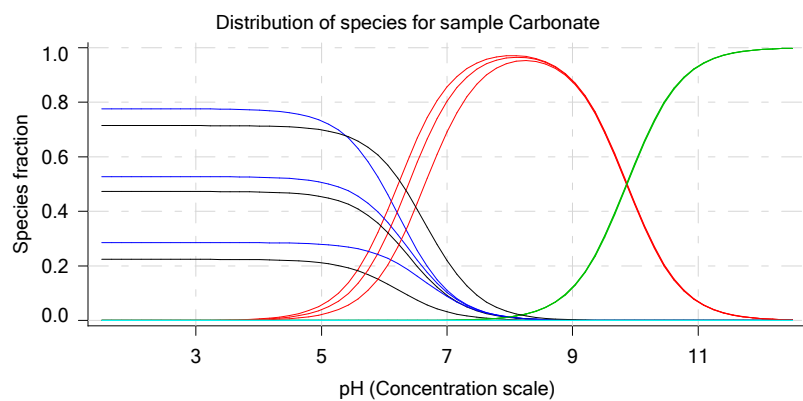
Graphs



Sample name: **M02_octanol**
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 Assay ID: **17L-14020**
 Filename: **G:\OpenLab_PFA_Sirius-T3-1\Sirius-T3-1\Data2017\17L-14020_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **12/14/2017 9:40:49 PM**
 Analyst: **Dorothy Levorse**
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Graphs (continued)



Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **17L-14020**
 Filename: **G:\OpenLab_PFA_Sirius-T3-1\Sirius-T3-1\Data2017\17L-14020_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **12/14/2017 9:40:49 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

pH-metric high logP Titration 1 of 3 17L-14020 Points 1 to 14

Overall results

RMSD 0.035
 Average ionic strength 0.158 M
 Average temperature 24.8°C
 Partition ratio 0.0935 : 1
 Analyte concentration range 3669.1 µM to 3783.1 µM
 Total points considered 14 of 14

Warnings and errors

Errors None
 Warnings None

Four-Plus parameters

Alpha 0.156 12/14/2017 9:40:49 PM C:\Sirius_T3\17L-14015_Blank standardisation.t3r
 S 0.9945 12/14/2017 9:40:49 PM C:\Sirius_T3\17L-14015_Blank standardisation.t3r
 jH 0.6 12/14/2017 9:40:49 PM C:\Sirius_T3\17L-14015_Blank standardisation.t3r
 jOH -0.7 12/14/2017 9:40:49 PM C:\Sirius_T3\17L-14015_Blank standardisation.t3r

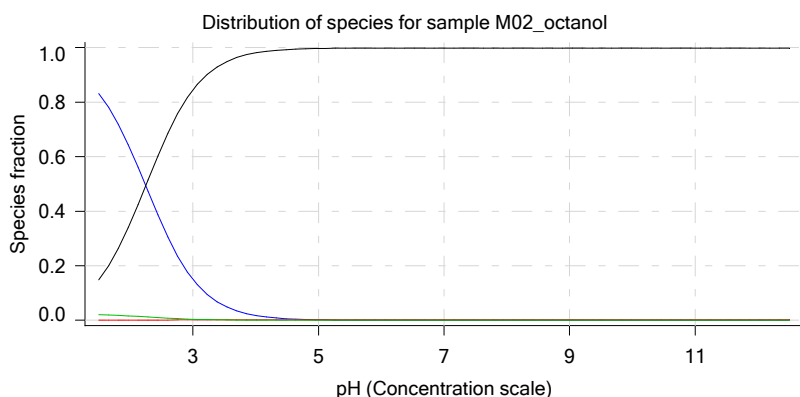
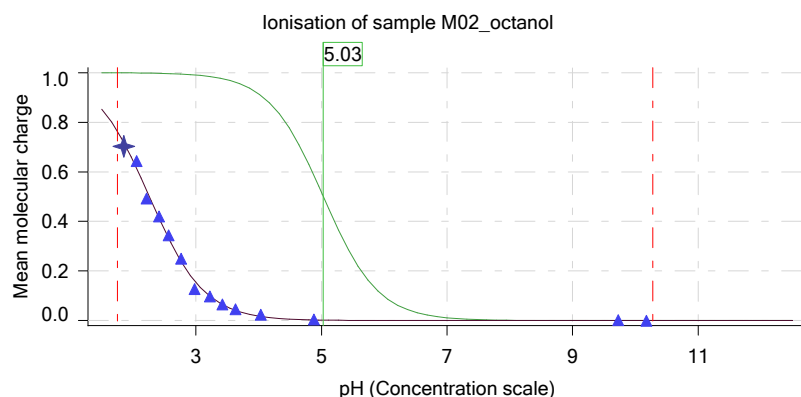
Titrants

0.50 M HCl 1.001830 12/14/2017 9:40:49 PM C:\Sirius_T3\17L-14015_Blank standardisation.t3r
 0.50 M KOH 1.010240 12/14/2017 9:40:49 PM C:\Sirius_T3\17L-11009_KHP_Base standardisation using KHP.t3r

Sample

M02_octanol concentration factor 0.941
 Base pKa 1 5.03
 logP (XH +) -0.57
 logP (neutral X) 3.81

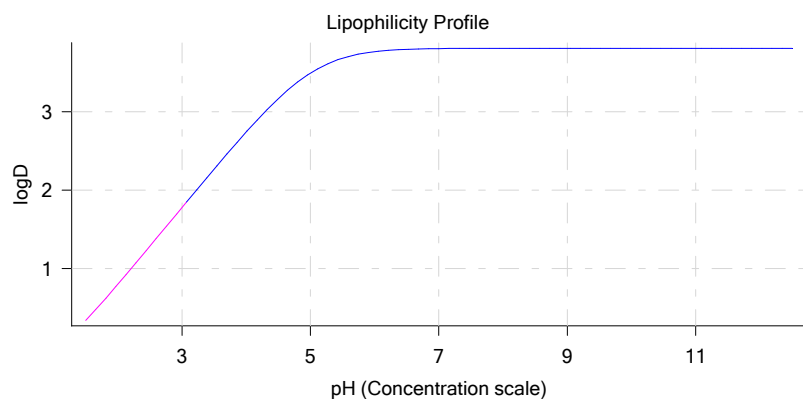
Sample graphs



Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **17L-14020**
 Filename: **G:\OpenLab_PFA_Sirius-T3-1\Sirius-T3-1\Data2017\17L-14020_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **12/14/2017 9:40:49 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**



Sample graphs (continued)



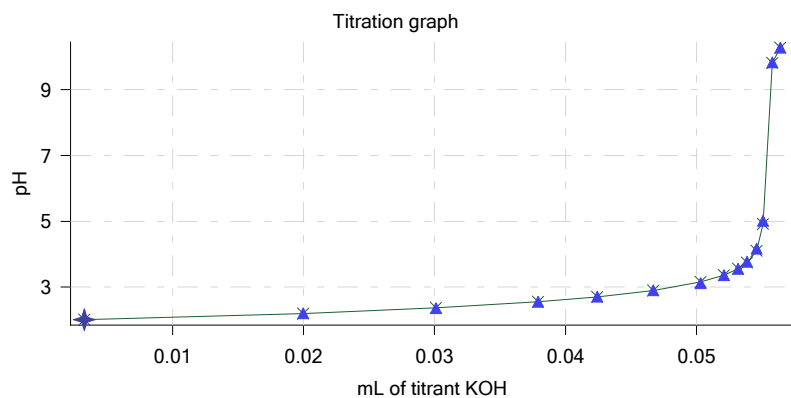
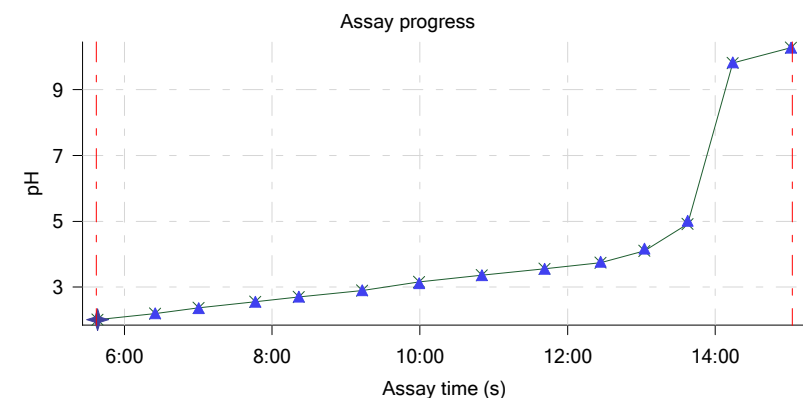
Sample logD and percent species

pH	M02_octanol logD	M02_octanol M02_octanolH	M02_octanol M02_octanolH	M02_octanol M02_octanolH*	M02_octanol M02_octanol*	Comment
1.000	-0.06	92.45 %	0.01 %	2.33 %	5.21 %	Stomach pH
1.200	0.09	89.71 %	0.01 %	2.26 %	8.02 %	
2.000	0.80	62.89 %	0.06 %	1.58 %	35.46 %	
3.000	1.78	14.99 %	0.14 %	0.38 %	84.50 %	
4.000	2.74	1.74 %	0.16 %	0.04 %	98.05 %	
5.000	3.49	0.18 %	0.16 %	0.00 %	99.65 %	Blood pH
6.000	3.77	0.02 %	0.17 %	0.00 %	99.82 %	
6.500	3.80	0.01 %	0.17 %	0.00 %	99.83 %	
7.000	3.81	0.00 %	0.17 %	0.00 %	99.83 %	
7.400	3.81	0.00 %	0.17 %	0.00 %	99.83 %	
8.000	3.81	0.00 %	0.17 %	0.00 %	99.83 %	
9.000	3.81	0.00 %	0.17 %	0.00 %	99.83 %	
10.000	3.81	0.00 %	0.17 %	0.00 %	99.83 %	
11.000	3.81	0.00 %	0.17 %	0.00 %	99.83 %	
12.000	3.81	0.00 %	0.17 %	0.00 %	99.83 %	

Carbonate and acidity

 Carbonate 0.079 mM
 Acidity error 0.007 mM

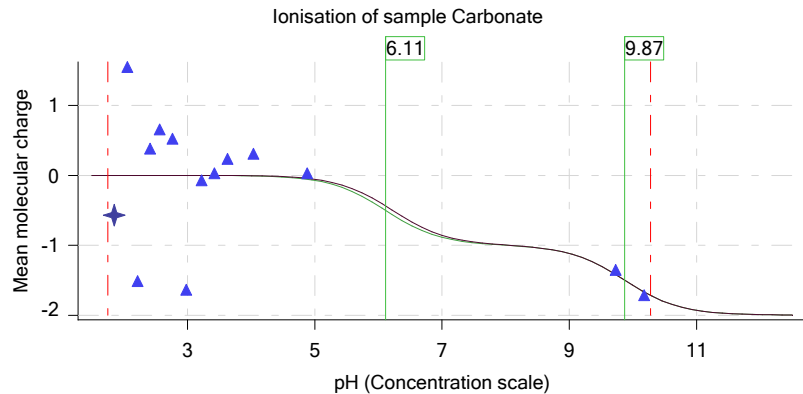
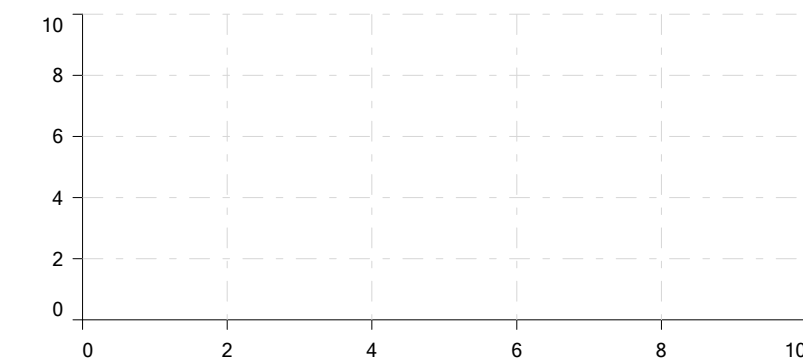
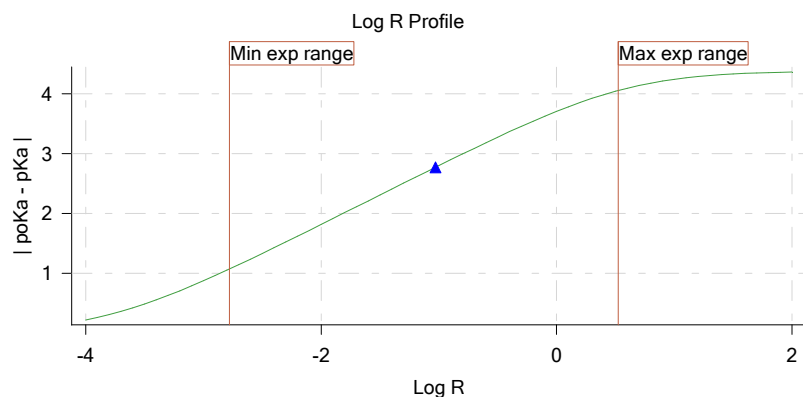
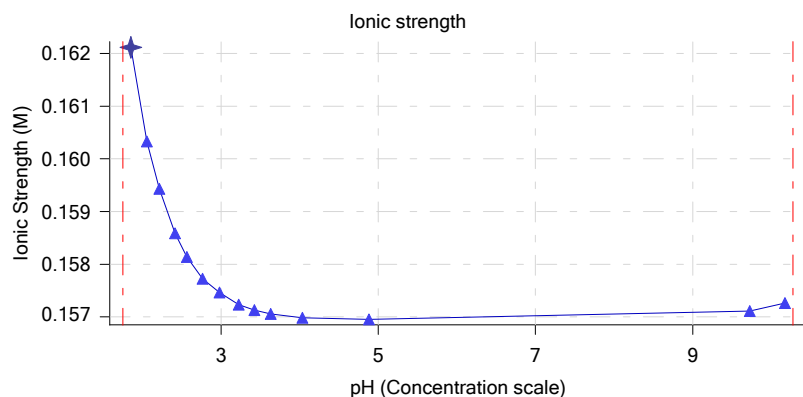
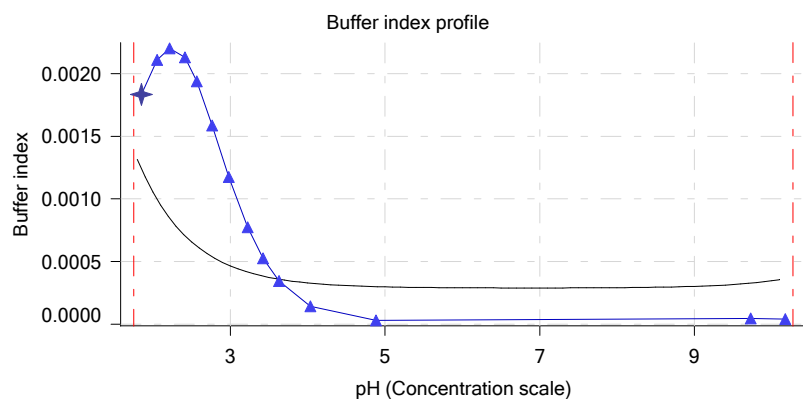
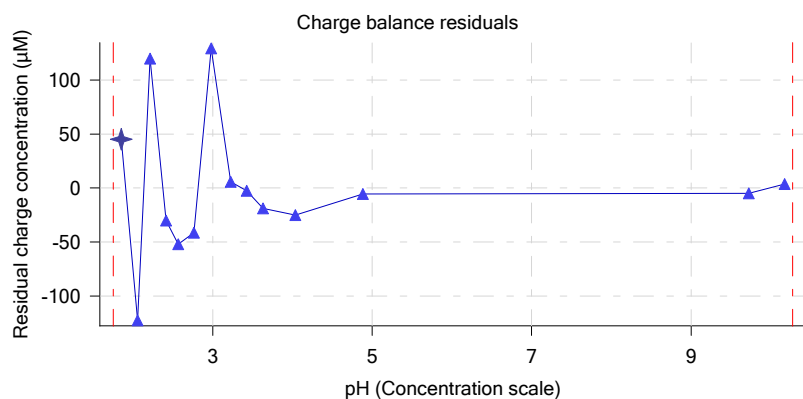
Other graphs



Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **17L-14020**
 Filename: **G:\OpenLab_PFA_Sirius-T3-1\Sirius-T3-1\Data2017\17L-14020_M02_octanol_pH-metric high logP.t3r**

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Other graphs (continued)



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 Filename: **G:\OpenLab_PFA_Sirius-T3-1\Sirius-T3-1\Data2017\17L-14020_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **12/14/2017 9:40:49 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

pH-metric high logP Titration 2 of 3 17L-14020 Points 15 to 31

Overall results

RMSD 0.353
 Average ionic strength 0.165 M
 Average temperature 24.9°C
 Partition ratio 0.2903 : 1
 Analyte concentration range 2895.7 µM to 2976.2 µM
 Total points considered 17 of 17

Warnings and errors

Errors None
 Warnings None

Four-Plus parameters

Alpha 0.156 12/14/2017 9:40:49 PM C:\Sirius_T3\17L-14015_Blank standardisation.t3r
 S 0.9945 12/14/2017 9:40:49 PM C:\Sirius_T3\17L-14015_Blank standardisation.t3r
 jH 0.6 12/14/2017 9:40:49 PM C:\Sirius_T3\17L-14015_Blank standardisation.t3r
 jOH -0.7 12/14/2017 9:40:49 PM C:\Sirius_T3\17L-14015_Blank standardisation.t3r

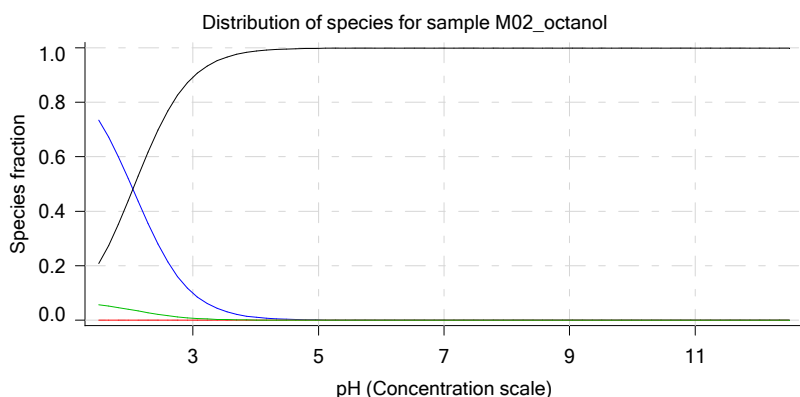
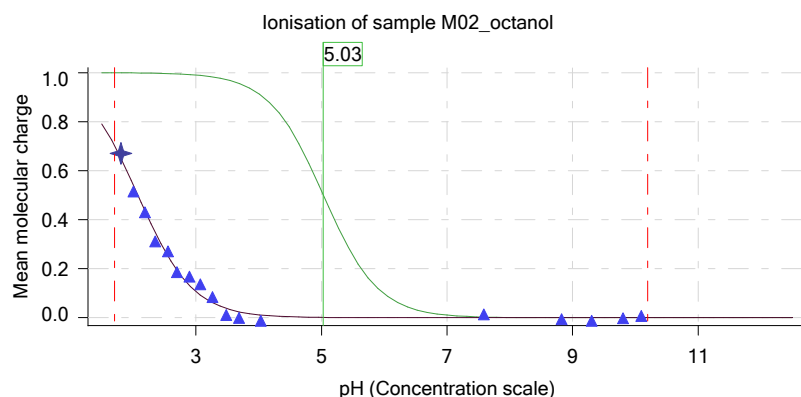
Titrants

0.50 M HCl 1.001830 12/14/2017 9:40:49 PM C:\Sirius_T3\17L-14015_Blank standardisation.t3r
 0.50 M KOH 1.010240 12/14/2017 9:40:49 PM C:\Sirius_T3\17L-11009_KHP_Base standardisation using KHP.t3r

Sample

M02_octanol concentration factor 0.825
 Base pKa 1 5.03
 logP (XH +) -0.57
 logP (neutral X) 3.52

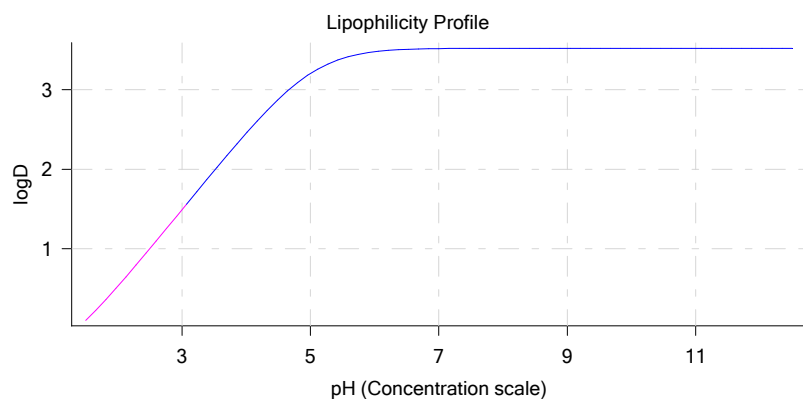
Sample graphs



Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **17L-14020**
 Filename: **G:\OpenLab_PFA_Sirius-T3-1\Sirius-T3-1\Data2017\17L-14020_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **12/14/2017 9:40:49 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Sample graphs (continued)



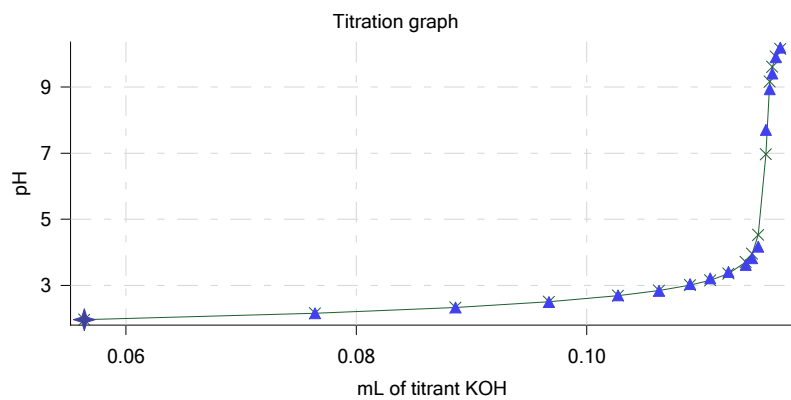
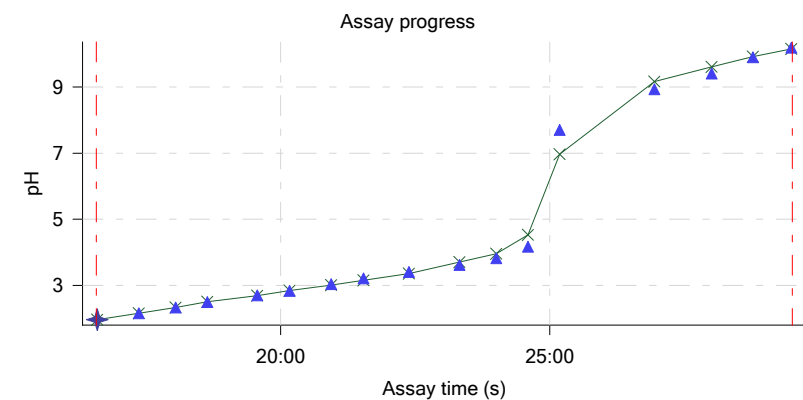
Sample logD and percent species

pH	M02_octanol logD	M02_octanol M02_octanolH	M02_octanol M02_octanolH	M02_octanol M02_octanolH*	M02_octanol M02_octanol*	Comment
1.000	-0.24	85.58 %	0.01 %	6.69 %	7.72 %	Stomach pH
1.200	-0.12	81.88 %	0.01 %	6.40 %	11.71 %	
2.000	0.53	50.46 %	0.05 %	3.94 %	45.55 %	
3.000	1.49	9.89 %	0.09 %	0.77 %	89.25 %	
4.000	2.45	1.09 %	0.10 %	0.09 %	98.72 %	
5.000	3.21	0.11 %	0.10 %	0.01 %	99.78 %	Blood pH
6.000	3.48	0.01 %	0.10 %	0.00 %	99.88 %	
6.500	3.51	0.00 %	0.10 %	0.00 %	99.89 %	
7.000	3.52	0.00 %	0.10 %	0.00 %	99.90 %	
7.400	3.52	0.00 %	0.10 %	0.00 %	99.90 %	
8.000	3.52	0.00 %	0.10 %	0.00 %	99.90 %	
9.000	3.52	0.00 %	0.10 %	0.00 %	99.90 %	
10.000	3.52	0.00 %	0.10 %	0.00 %	99.90 %	
11.000	3.52	0.00 %	0.10 %	0.00 %	99.90 %	
12.000	3.52	0.00 %	0.10 %	0.00 %	99.90 %	

Carbonate and acidity

Carbonate 0.196 mM
 Acidity error 0.060 mM

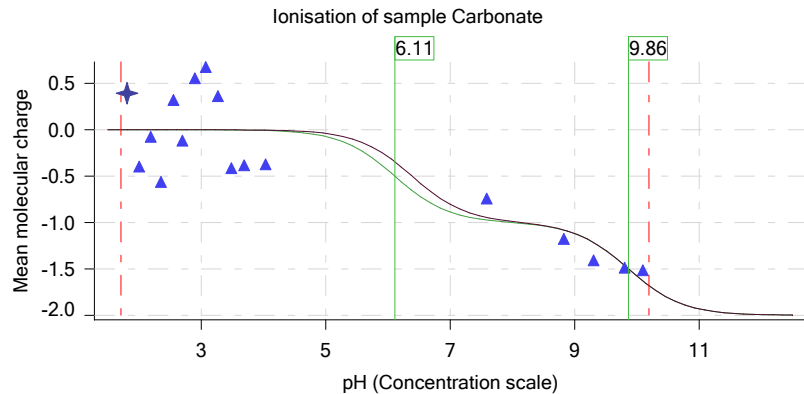
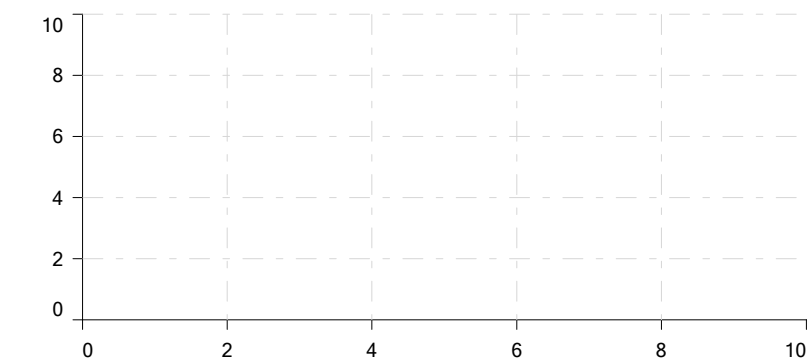
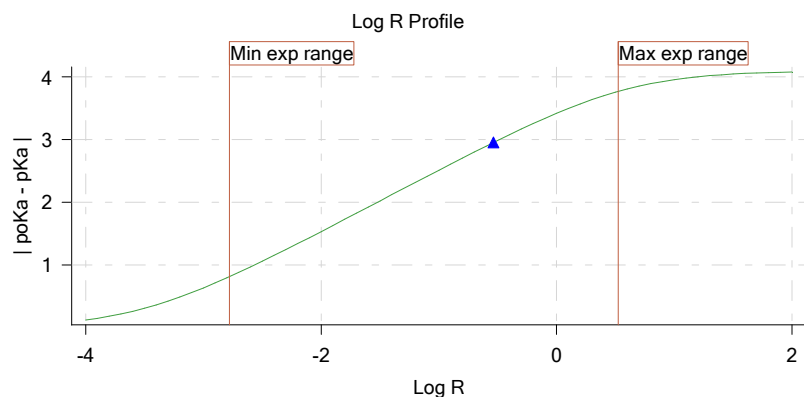
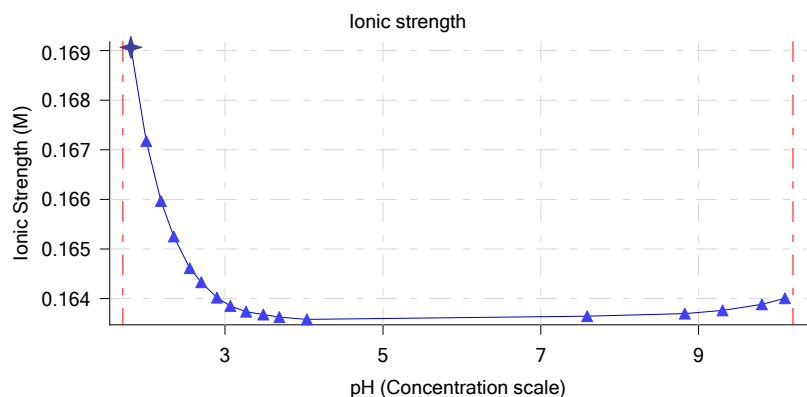
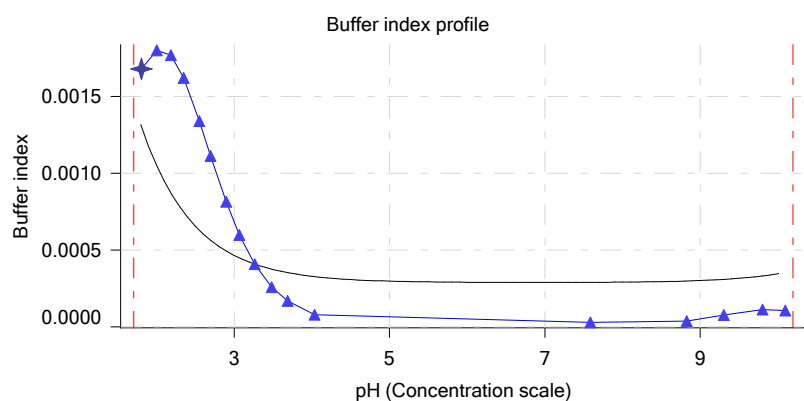
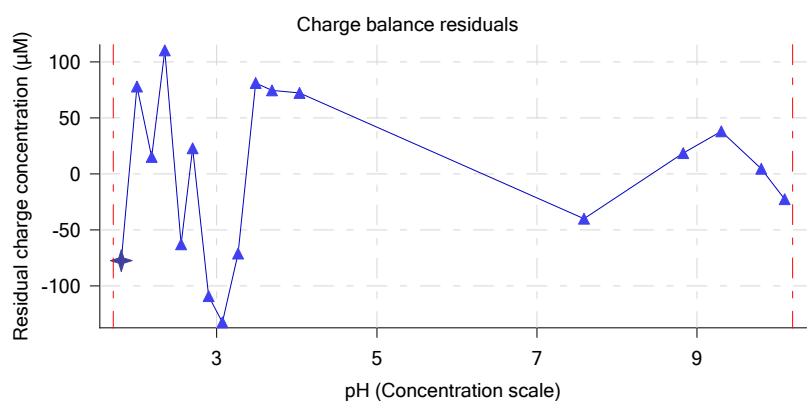
Other graphs



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 Filename: **G:\OpenLab_PFA_Sirius-T3-1\Sirius-T3-1\Data2017\17L-14020_M02_octanol_pH-metric high logP.t3r**

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Other graphs (continued)



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Experiment start time: **12/14/2017 9:40:49 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

pH-metric high logP Titration 3 of 3 17L-14020 Points 32 to 50

Overall results

RMSD 0.347
 Average ionic strength 0.170 M
 Average temperature 25.0°C
 Partition ratio 0.8090 : 1
 Analyte concentration range 1923.2 µM to 1961.3 µM
 Total points considered 12 of 19

Warnings and errors

Errors None
 Warnings Sample concentration factor out of range

Four-Plus parameters

Alpha 0.156 12/14/2017 9:40:49 PM C:\Sirius_T3\17L-14015_Blank standardisation.t3r
 S 0.9945 12/14/2017 9:40:49 PM C:\Sirius_T3\17L-14015_Blank standardisation.t3r
 jH 0.6 12/14/2017 9:40:49 PM C:\Sirius_T3\17L-14015_Blank standardisation.t3r
 jOH -0.7 12/14/2017 9:40:49 PM C:\Sirius_T3\17L-14015_Blank standardisation.t3r

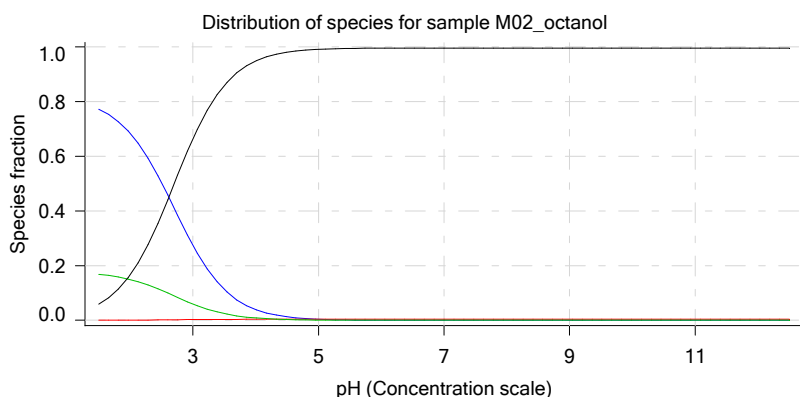
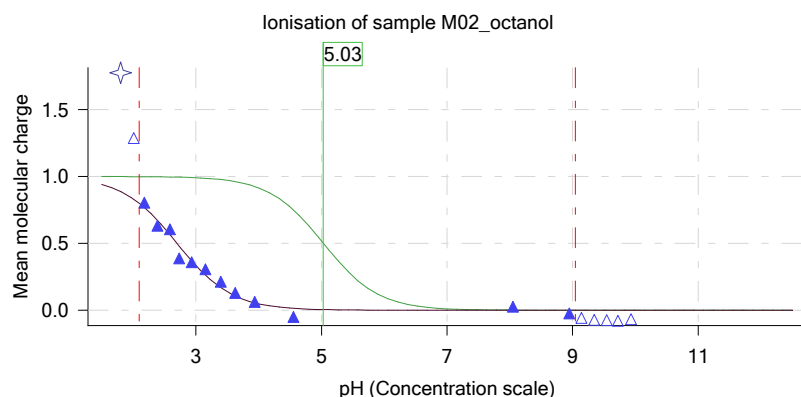
Titrants

0.50 M HCl 1.001830 12/14/2017 9:40:49 PM C:\Sirius_T3\17L-14015_Blank standardisation.t3r
 0.50 M KOH 1.010240 12/14/2017 9:40:49 PM C:\Sirius_T3\17L-11009_KHP_Base standardisation using KHP.t3r

Sample

M02_octanol concentration factor 0.307
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 logP (XH +) -0.57
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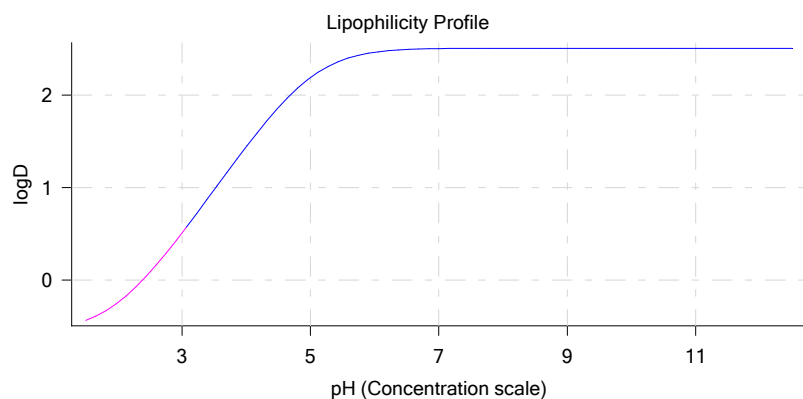
Sample graphs



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 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**



Sample graphs (continued)



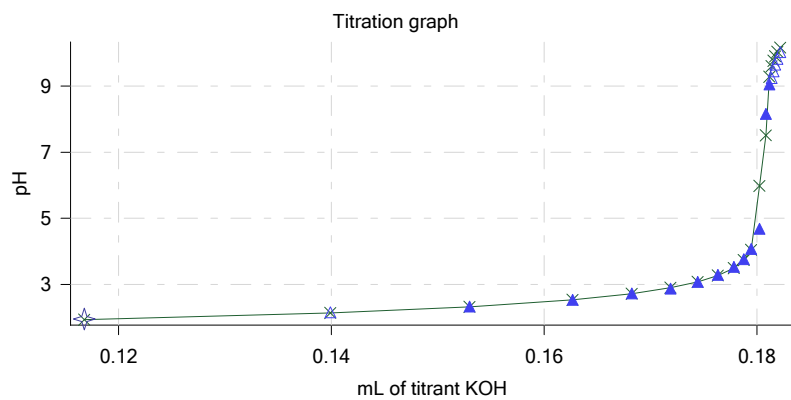
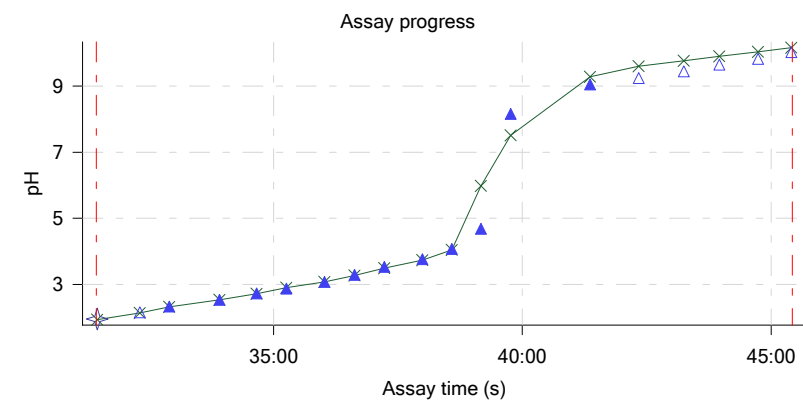
Sample logD and percent species

pH	M02_octanol logD	M02_octanol M02_octanolH	M02_octanol M02_octanolH	M02_octanol M02_octanolH*	M02_octanol M02_octanol*	Comment
1.000	-0.52	80.51 %	0.01 %	17.53 %	1.96 %	Stomach pH
1.200	-0.50	79.59 %	0.01 %	17.33 %	3.07 %	
2.000	-0.24	68.41 %	0.06 %	14.90 %	16.63 %	
3.000	0.51	27.34 %	0.26 %	5.95 %	66.45 %	
4.000	1.44	3.90 %	0.36 %	0.85 %	94.88 %	
5.000	2.19	0.41 %	0.38 %	0.09 %	99.12 %	Blood pH
6.000	2.46	0.04 %	0.38 %	0.01 %	99.57 %	
6.500	2.49	0.01 %	0.38 %	0.00 %	99.60 %	
7.000	2.50	0.00 %	0.38 %	0.00 %	99.61 %	
7.400	2.51	0.00 %	0.38 %	0.00 %	99.62 %	
8.000	2.51	0.00 %	0.38 %	0.00 %	99.62 %	
9.000	2.51	0.00 %	0.38 %	0.00 %	99.62 %	
10.000	2.51	0.00 %	0.38 %	0.00 %	99.62 %	
11.000	2.51	0.00 %	0.38 %	0.00 %	99.62 %	
12.000	2.51	0.00 %	0.38 %	0.00 %	99.62 %	

Carbonate and acidity

 Carbonate 0.220 mM
 Acidity error 0.620 mM

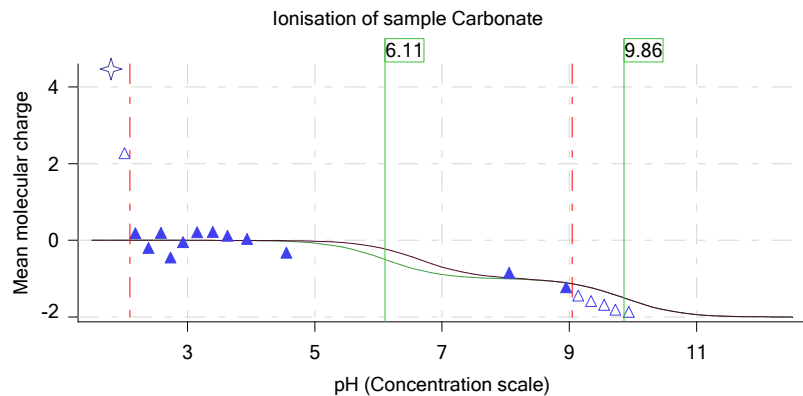
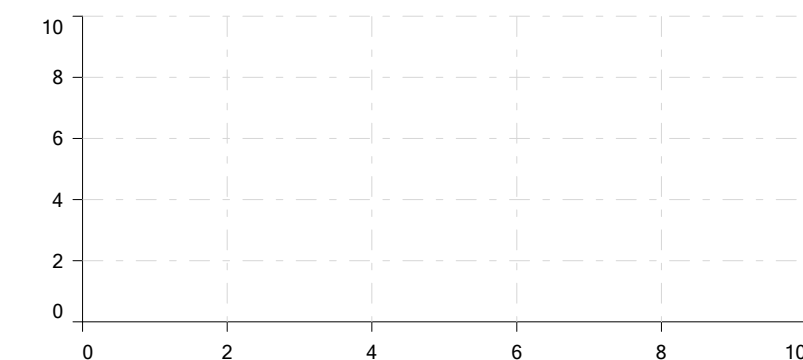
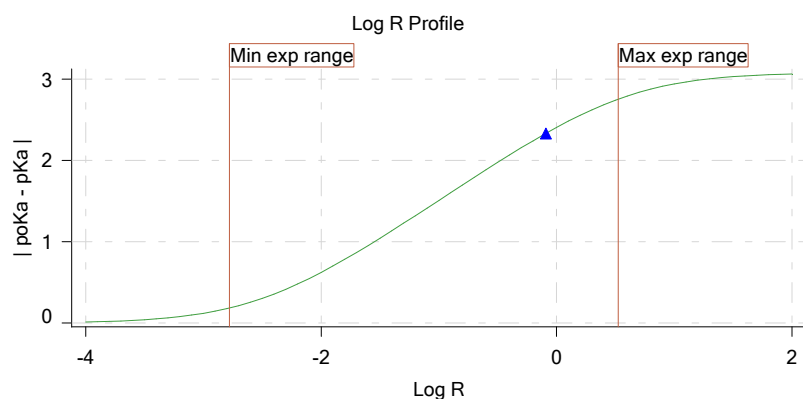
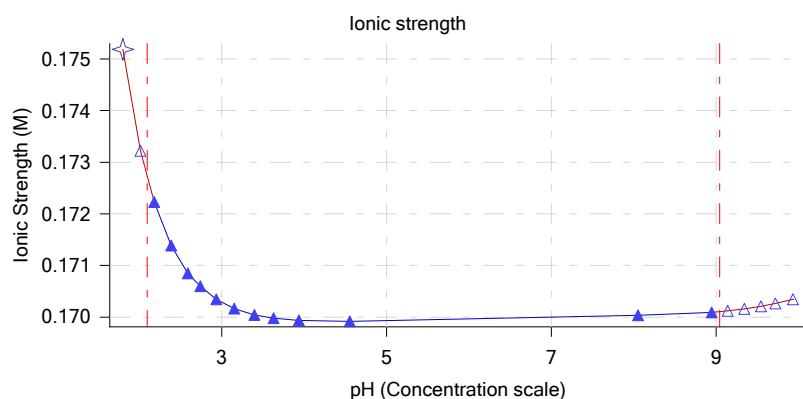
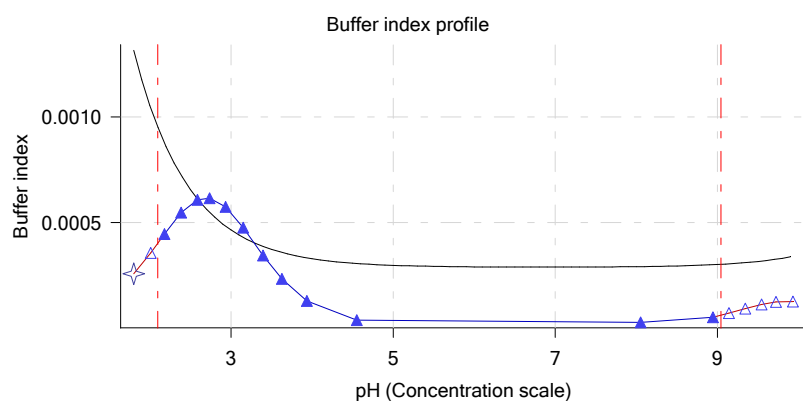
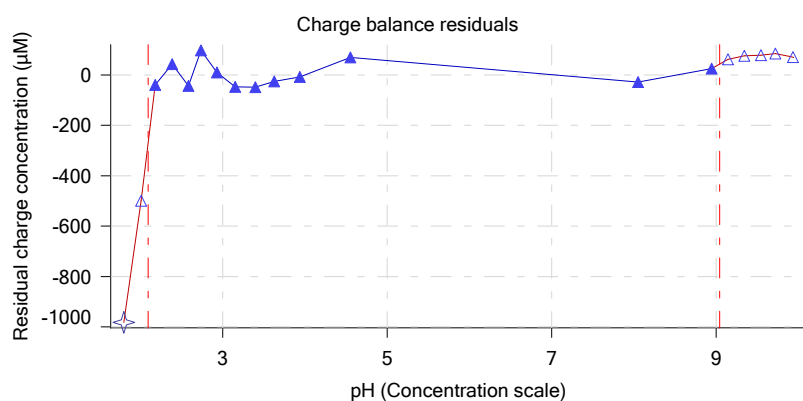
Other graphs



Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **17L-14020**
 Filename: **G:\OpenLab_PFA_Sirius-T3-1\Sirius-T3-1\Data2017\17L-14020_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **12/14/2017 9:40:49 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Other graphs (continued)



Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **17L-14020**
 Filename: **G:\OpenLab_PFA_Sirius-T3-1\Sirius-T3-1\Data2017\17L-14020_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **12/14/2017 9:40:49 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M02_octanol	12/6/2017 5:20:03 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001870 g	12/14/2017 4:31:54 PM	User entered value
Formula weight	289.26 g/mol	12/6/2017 5:20:03 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	289.26	12/6/2017 5:20:03 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	12/6/2017 5:20:03 PM	User entered value
Sample is a	Base	12/6/2017 5:20:03 PM	User entered value
pKa 1	5.03	12/6/2017 5:20:03 PM	User entered value
logp (XH +)	-0.57	12/14/2017 3:31:39 PM	User entered value
logP (neutral X)	0.94	12/14/2017 3:31:32 PM	User entered value

Events

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
2:38.7	Initial pH = 6.57									
5:38.2	Data point 1	1.50000 mL	0.05560 mL	0.00327 mL	0.15000 mL	2.007	0.00139	0.03368	0.00037	10.5 s
6:24.9	Data point 2	1.50000 mL	0.05560 mL	0.01997 mL	0.15000 mL	2.206	-0.00747	0.39684	0.00059	10.0 s
7:00.4	Data point 3	1.50000 mL	0.05560 mL	0.03010 mL	0.15000 mL	2.363	-0.00559	0.19734	0.00062	10.0 s
7:46.3	Data point 4	1.50000 mL	0.05560 mL	0.03791 mL	0.15000 mL	2.558	-0.01487	0.86800	0.00079	10.0 s
8:21.8	Data point 5	1.50000 mL	0.05560 mL	0.04243 mL	0.15000 mL	2.710	-0.00425	0.44243	0.00032	10.5 s
9:13.3	Data point 6	1.50000 mL	0.05560 mL	0.04671 mL	0.15000 mL	2.907	-0.00837	0.81909	0.00046	10.5 s
9:59.6	Data point 7	1.50000 mL	0.05560 mL	0.05031 mL	0.15000 mL	3.120	-0.01056	0.38594	0.00084	10.0 s
10:50.5	Data point 8	1.50000 mL	0.05560 mL	0.05209 mL	0.15000 mL	3.363	-0.01094	0.53189	0.00074	10.0 s
11:41.4	Data point 9	1.50000 mL	0.05560 mL	0.05318 mL	0.15000 mL	3.562	-0.00971	0.40417	0.00075	10.0 s
12:27.0	Data point 10	1.50000 mL	0.05560 mL	0.05386 mL	0.15000 mL	3.767	-0.01049	0.64757	0.00064	10.0 s
13:02.4	Data point 11	1.50000 mL	0.05560 mL	0.05459 mL	0.15000 mL	4.170	-0.00778	0.67581	0.00047	10.0 s
13:37.7	Data point 12	1.50000 mL	0.05560 mL	0.05508 mL	0.15000 mL	5.011	0.00369	0.07856	0.00065	11.0 s
14:14.1	Data point 13	1.50000 mL	0.05560 mL	0.05579 mL	0.15000 mL	9.827	-0.01899	0.90855	0.00098	17.0 s
15:01.6	Data point 14	1.50000 mL	0.05560 mL	0.05640 mL	0.15000 mL	10.274	-0.01908	0.91794	0.00098	17.0 s
16:35.5	Data point 15	1.50000 mL	0.11580 mL	0.05640 mL	0.50000 mL	1.964	-0.00642	0.19348	0.00072	10.0 s
17:21.8	Data point 16	1.50000 mL	0.11580 mL	0.07641 mL	0.50000 mL	2.155	-0.01440	0.57008	0.00094	15.5 s
18:03.0	Data point 17	1.50000 mL	0.11580 mL	0.08862 mL	0.50000 mL	2.336	-0.01761	0.86346	0.00094	10.0 s
18:38.5	Data point 18	1.50000 mL	0.11580 mL	0.09671 mL	0.50000 mL	2.499	-0.01747	0.85915	0.00093	14.5 s
19:34.1	Data point 19	1.50000 mL	0.11580 mL	0.10271 mL	0.50000 mL	2.699	-0.01738	0.83571	0.00094	10.5 s
20:10.1	Data point 20	1.50000 mL	0.11580 mL	0.10626 mL	0.50000 mL	2.841	-0.01842	0.94159	0.00094	10.5 s
20:56.5	Data point 21	1.50000 mL	0.11580 mL	0.10896 mL	0.50000 mL	3.039	-0.00529	0.32126	0.00046	10.5 s
21:32.5	Data point 22	1.50000 mL	0.11580 mL	0.11070 mL	0.50000 mL	3.210	-0.01298	0.72113	0.00075	10.0 s
22:23.3	Data point 23	1.50000 mL	0.11580 mL	0.11230 mL	0.50000 mL	3.404	-0.01202	0.61736	0.00075	10.0 s
23:19.3	Data point 24	1.50000 mL	0.11580 mL	0.11381 mL	0.50000 mL	3.623	-0.00105	0.02529	0.00033	10.5 s
24:00.4	Data point 25	1.50000 mL	0.11580 mL	0.11435 mL	0.50000 mL	3.825	-0.01396	0.59332	0.00089	10.0 s
24:35.7	Data point 26	1.50000 mL	0.11580 mL	0.11486 mL	0.50000 mL	4.169	-0.00892	0.71187	0.00052	10.0 s
25:11.0	Data point 27	1.50000 mL	0.11580 mL	0.11555 mL	0.50000 mL	7.702	-0.10242	0.99687	0.00506	Timed out at 59.5 s
26:56.8	Data point 28	1.50000 mL	0.11580 mL	0.11588 mL	0.50000 mL	8.934	-0.01413	0.48746	0.00100	28.0 s
28:00.6	Data point 29	1.50000 mL	0.11580 mL	0.11611 mL	0.50000 mL	9.408	-0.01497	0.88842	0.00078	15.5 s
28:46.6	Data point 30	1.50000 mL	0.11580 mL	0.11642 mL	0.50000 mL	9.903	-0.01712	0.83019	0.00093	12.5 s
29:29.6	Data point 31	1.50000 mL	0.11580 mL	0.11679 mL	0.50000 mL	10.194	-0.01474	0.64645	0.00091	10.0 s
31:27.3	Data point 32	1.50000 mL	0.17935 mL	0.11679 mL	1.50000 mL	1.957	-0.01138	0.54149	0.00076	10.0 s
32:18.7	Data point 33	1.50000 mL	0.17935 mL	0.13991 mL	1.50000 mL	2.162	-0.00826	0.34190	0.00070	10.0 s
32:54.3	Data point 34	1.50000 mL	0.17935 mL	0.15299 mL	1.50000 mL	2.329	0.00841	0.21086	0.00090	19.5 s
33:54.9	Data point 35	1.50000 mL	0.17935 mL	0.16268 mL	1.50000 mL	2.533	-0.01444	0.56679	0.00095	19.0 s
34:39.5	Data point 36	1.50000 mL	0.17935 mL	0.16825 mL	1.50000 mL	2.729	-0.01081	0.59250	0.00069	10.5 s
35:15.5	Data point 37	1.50000 mL	0.17935 mL	0.17190 mL	1.50000 mL	2.879	0.00523	0.07679	0.00093	10.0 s
36:01.3	Data point 38	1.50000 mL	0.17935 mL	0.17444 mL	1.50000 mL	3.074	-0.01576	0.64444	0.00097	11.0 s
36:37.8	Data point 39	1.50000 mL	0.17935 mL	0.17634 mL	1.50000 mL	3.290	-0.01372	0.74324	0.00079	10.5 s



Assay Events

Sample name: **M02_octanol** Experiment start time: **12/14/2017 9:40:49 PM**
Assay name: **pH-metric high logP** Analyst: **Dorothy Levorse**
Assay ID: **17L-14020** Instrument ID: **T311053**
Filename: **G:\OpenLab_PFA_Sirius-T3-1\Sirius-T3-1\Data2017\17L-14020_M02_octanol_pH-metric high logP.t3r**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
37:13.7	Data point 40	1.50000 mL	0.17935 mL	0.17782 mL	1.50000 mL	3.534	-0.00886	0.57323	0.00058	10.0 s
37:59.4	Data point 41	1.50000 mL	0.17935 mL	0.17876 mL	1.50000 mL	3.765	-0.00909	0.36165	0.00075	10.0 s
38:34.8	Data point 42	1.50000 mL	0.17935 mL	0.17947 mL	1.50000 mL	4.071	-0.00570	0.25273	0.00056	10.0 s
39:10.1	Data point 43	1.50000 mL	0.17935 mL	0.18024 mL	1.50000 mL	4.684	-0.00391	0.12958	0.00054	10.5 s
39:46.0	Data point 44	1.50000 mL	0.17935 mL	0.18083 mL	1.50000 mL	8.163	-0.13728	0.99581	0.00680	Timed out at 59.5 s
41:21.6	Data point 45	1.50000 mL	0.17935 mL	0.18119 mL	1.50000 mL	9.052	-0.01846	0.83706	0.00100	23.0 s
42:20.2	Data point 46	1.50000 mL	0.17935 mL	0.18140 mL	1.50000 mL	9.247	-0.00723	0.15620	0.00090	19.0 s
43:14.9	Data point 47	1.50000 mL	0.17935 mL	0.18156 mL	1.50000 mL	9.446	-0.00873	0.24834	0.00086	12.0 s
43:57.4	Data point 48	1.50000 mL	0.17935 mL	0.18173 mL	1.50000 mL	9.647	-0.00896	0.20472	0.00098	11.0 s
44:44.1	Data point 49	1.50000 mL	0.17935 mL	0.18194 mL	1.50000 mL	9.822	0.00182	0.01449	0.00075	10.0 s
45:24.5	Data point 50	1.50000 mL	0.17935 mL	0.18220 mL	1.50000 mL	10.033	0.01248	0.45958	0.00091	15.0 s
45:48.4	Assay volumes	1.50000 mL	0.17935 mL	0.18220 mL	1.50000 mL					



Sample name: **M02_octanol** Experiment start time: **12/14/2017 9:40:49 PM**
Assay name: **pH-metric high logP** Analyst: **Dorothy Levorse**
Assay ID: **17L-14020** Instrument ID: **T311053**
Filename: **G:\OpenLab_PFA_Sirius-T3-1\Sirius-T3-1\Data2017\17L-14020_M02_octanol_pH-metric high logP.t3r**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Dorothy Levorse			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	10.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	Yes			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titration Pre-Dose				
Titration pre-dose	None			
Assay Medium				
ISA water volume	1.50 mL			
Water added	Automatic			
After water addition, stir for	5 seconds			
At a speed of	10%			
Partition solvent type	Octanol			
Partition volume	0.150 mL			
Partition solvent added	Automatic			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	No			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.350 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			
Titration 3				

Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **17L-14020**
 Filename: **G:\OpenLab_PFA_Sirius-T3-1\Sirius-T3-1\Data2017\17L-14020_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **12/14/2017 9:40:49 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	1.000 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.156	12/14/2017 9:40:49 PM	C:\Sirius_T3\17L-14015_Blank standardisation.t3r
Four-Plus S	0.9945	12/14/2017 9:40:49 PM	C:\Sirius_T3\17L-14015_Blank standardisation.t3r
Four-Plus jH	0.6	12/14/2017 9:40:49 PM	C:\Sirius_T3\17L-14015_Blank standardisation.t3r
Four-Plus jOH	-0.7	12/14/2017 9:40:49 PM	C:\Sirius_T3\17L-14015_Blank standardisation.t3r
Base concentration factor	1.010	12/14/2017 9:40:49 PM	C:\Sirius_T3\17L-11009_KHP_Base standardisation using KHP.t3r
Acid concentration factor	1.002	12/14/2017 9:40:49 PM	C:\Sirius_T3\17L-14015_Blank standardisation.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T311053		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1100253	3/31/2009 6:24:52 AM
Dispenser 0	Water		3/31/2009 6:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	10-10-2017	12/6/2017 10:48:42 AM
Dispenser 2	Acid		3/31/2009 6:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	12-6-2017	12/6/2017 10:50:31 AM
Dispenser 1	Base		3/31/2009 6:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	09-22-17	11/27/2017 10:30:45 AM
Dispenser 5	Cosolvent		3/31/2009 6:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 6:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	9-26-17	12/11/2017 11:29:08 AM
Port B	Cyclohexane		10/19/2017 3:11:05 PM
Port C	MeCN (50%, 0.15 M KCl)	10-30-17	11/27/2017 10:21:50 AM
Dispenser 3	Buffer		8/3/2010 6:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane		12/6/2017 10:50:59 AM
Dispenser 6	Octanol		10/22/2010 11:52:43 AM

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **17L-14020**
Filename: **G:\OpenLab_PFA_Sirius-T3-1\Sirius-T3-1\Data2017\17L-14020_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **12/14/2017 9:40:49 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	9-14-17	12/11/2017 11:32:26 AM
Titration		T3TM1100153	3/31/2009 6:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0769	8/15/2017 10:21:54 AM
E0 calibration	-5.35 mV		12/14/2017 9:41:17 PM
Filling solution	3M KCl	KCL095	12/14/2017 3:53:24 PM
Liquids			
Wash 1	50% IPA:50% Water		12/14/2017 3:56:50 PM
Wash 2	0.5% Triton X-100 in H2O		12/14/2017 3:56:52 PM
Buffer position 1	pH7 Wash		12/14/2017 3:56:54 PM
Buffer position 2	pH 7		12/14/2017 3:56:57 PM
Storage position			12/14/2017 3:57:36 PM
Wash water	6.6e+003 mL	12-11-2017	12/11/2017 3:16:20 PM
Waste	3.5e+003 mL		12/11/2017 3:16:25 PM
Temperature controller			8/5/2010 7:35:13 AM
Turbidity detector			3/31/2009 6:24:45 AM
Spectrometer		072390	11/23/2010 12:22:28 PM
Dip probe		11086	
Wavelength coefficient A0	185.563		
Wavelength coefficient A1	2.17439		
Wavelength coefficient A2	-0.000285622		
Total lamp lit time	644:54:39		11/23/2010 12:22:28 PM
Calibrated on	12/4/2017 11:26:25 AM		
Integration time	11		
Scans averaged	10		
Autoloader		T3AL1100237	11/10/2015 10:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titration tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		



Assay Settings

Sample name: **M02_octanol** Experiment start time: **12/14/2017 9:40:49 PM**
Assay name: **pH-metric high logP** Analyst: **Dorothy Levorse**
Assay ID: **17L-14020** Instrument ID: **T311053**
Filename: **G:\OpenLab_PFA_Sirius-T3-1\Sirius-T3-1\Data2017\17L-14020_M02_octanol_pH-metric high logP.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00